

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082418\
 Data File : BF108479.D
 Acq On : 24 Aug 2018 22:29
 Operator : JU/SJ
 Sample : J4581-17
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q3-D1

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.372	3	6	18	rVB	888121	1177703	30.76%	3.458%
2	4.778	412	415	419	rBV	39518	45062	1.18%	0.132%
3	5.254	492	496	505	rVB	137395	176289	4.60%	0.518%
4	5.631	555	560	563	rBV	3254571	3135141	81.88%	9.206%
5	6.625	723	729	732	rBV	3291269	3400816	88.82%	9.986%
6	6.772	749	754	757	rBV	3590013	3359414	87.74%	9.864%
7	6.996	789	792	796	rBV	1002755	880210	22.99%	2.585%
8	7.154	815	819	823	rBV	2854382	2570168	67.12%	7.547%
9	7.560	883	888	892	rBV	2040316	2261923	59.07%	6.642%
10	8.284	1006	1011	1014	rBV	1162070	1098805	28.70%	3.226%
11	9.354	1188	1193	1197	rBV	4089369	3828943	100.00%	11.243%
12	9.748	1256	1260	1263	rBV	1062421	928479	24.25%	2.726%
13	10.042	1306	1310	1314	rBV	1505171	1269523	33.16%	3.728%
14	10.836	1440	1445	1458	rBV	2666858	2526955	66.00%	7.420%
15	11.536	1560	1564	1567	rBV	1393403	1253292	32.73%	3.680%
16	12.042	1646	1650	1653	rBV	114188	107025	2.80%	0.314%
17	12.754	1767	1771	1775	rBV	63938	57159	1.49%	0.168%
18	12.989	1809	1811	1815	rVB	61995	58033	1.52%	0.170%
19	13.125	1829	1834	1837	rBV	3448459	3137854	81.95%	9.214%
20	13.672	1923	1927	1930	rBV2	43805	42952	1.12%	0.126%
21	14.001	1980	1983	1985	rBV	56263	46591	1.22%	0.137%
22	14.066	1988	1994	1999	rBV6	32733	85543	2.23%	0.251%
23	14.189	2010	2015	2019	rBV	926868	838854	21.91%	2.463%
24	14.319	2031	2037	2040	rBV	51157	49141	1.28%	0.144%
25	14.624	2085	2089	2094	rBV	59307	56522	1.48%	0.166%
26	14.936	2138	2142	2149	rBV2	363246	441682	11.54%	1.297%
27	15.030	2155	2158	2164	rVB	213829	216737	5.66%	0.636%
28	15.307	2202	2205	2210	rVB2	58504	73014	1.91%	0.214%
29	15.742	2271	2279	2292	rBV	589246	870787	22.74%	2.557%
30	16.189	2351	2355	2361	rVB	38613	61568	1.61%	0.181%

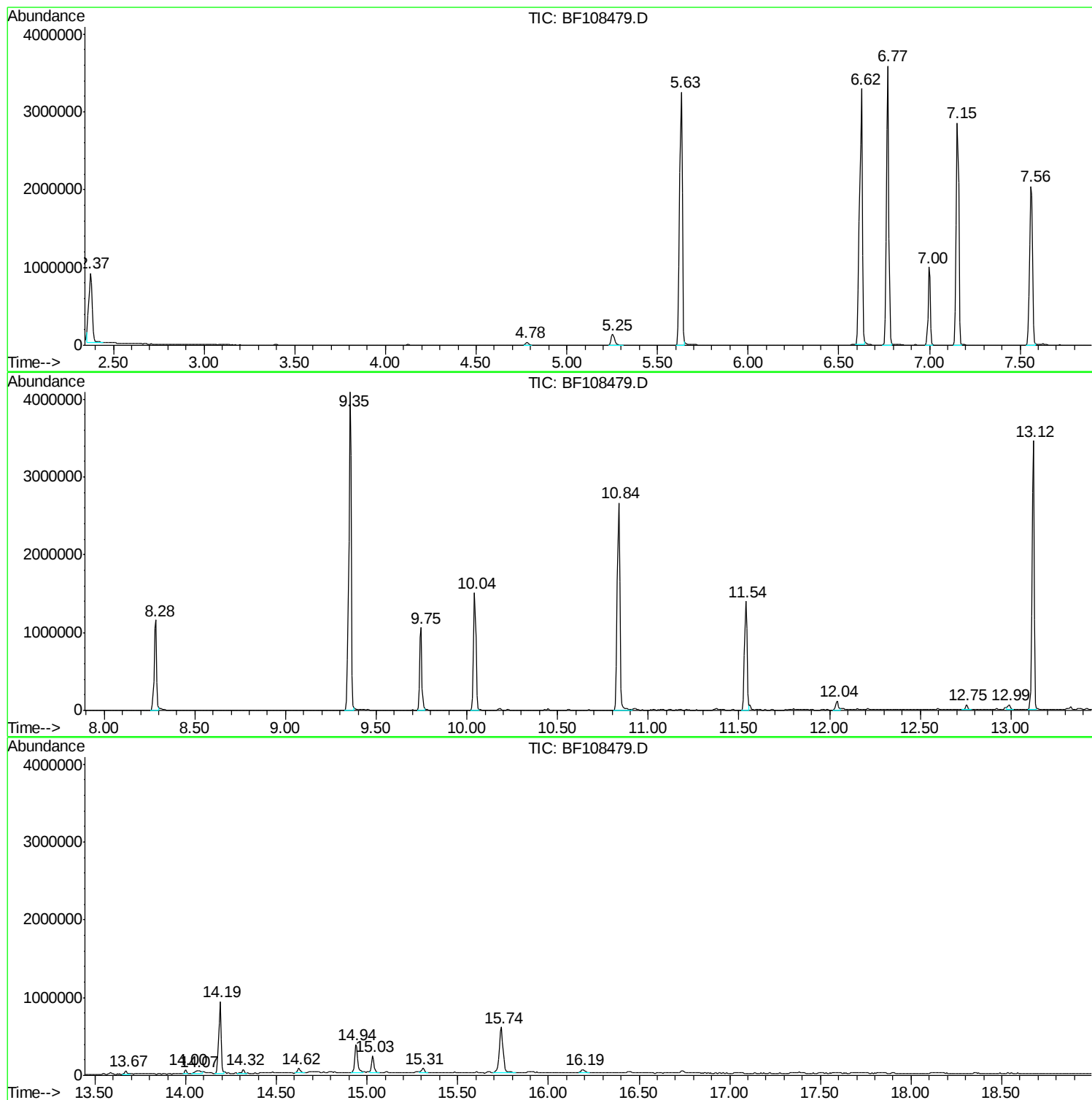
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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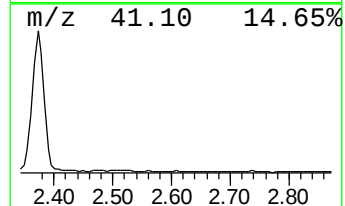
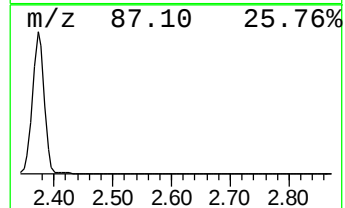
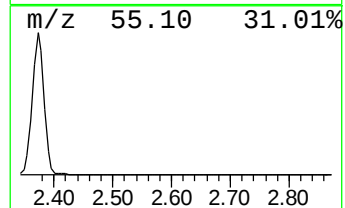
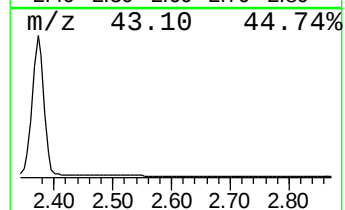
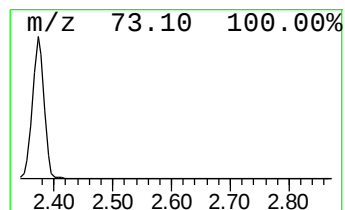
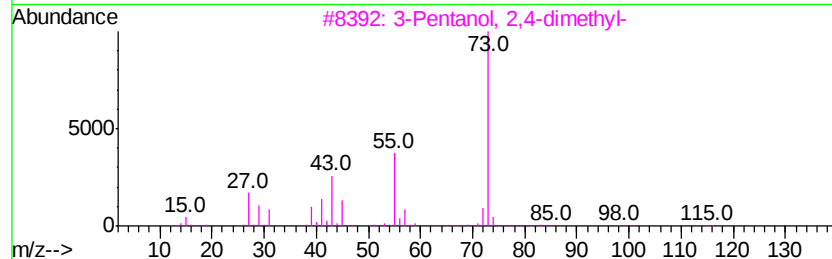
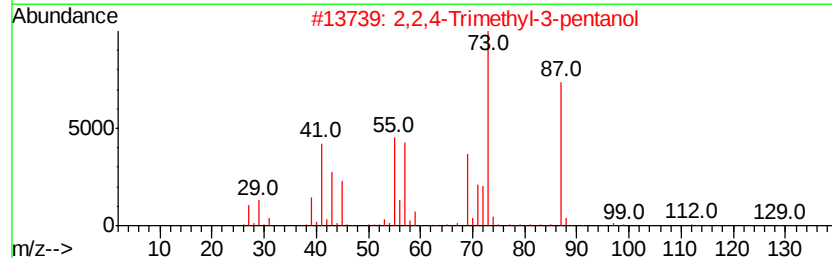
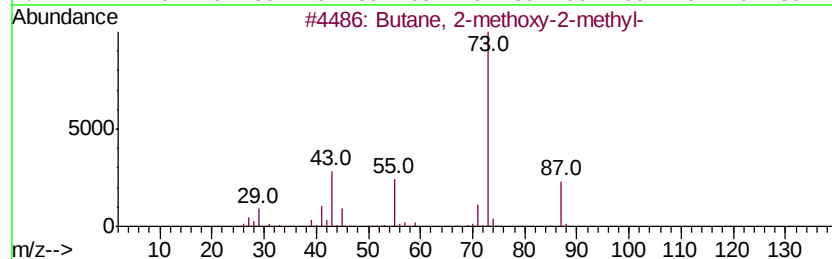
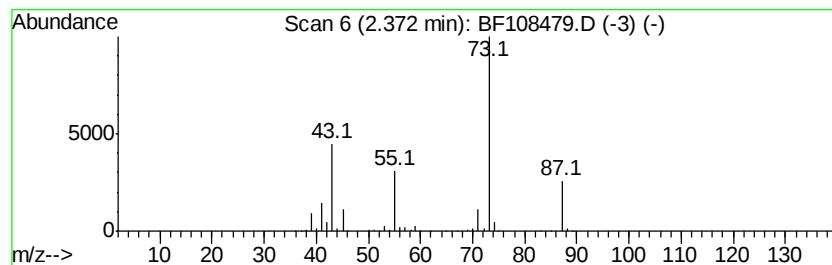
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	26.76 ng	1177700	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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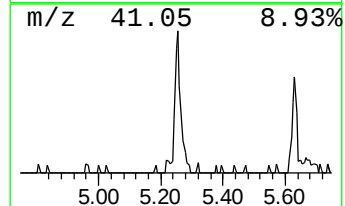
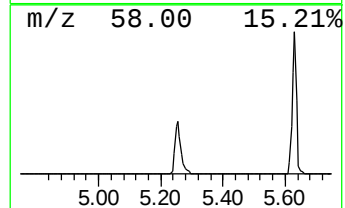
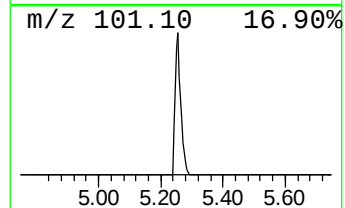
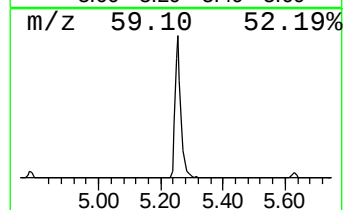
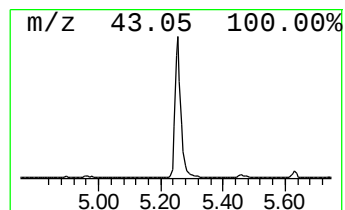
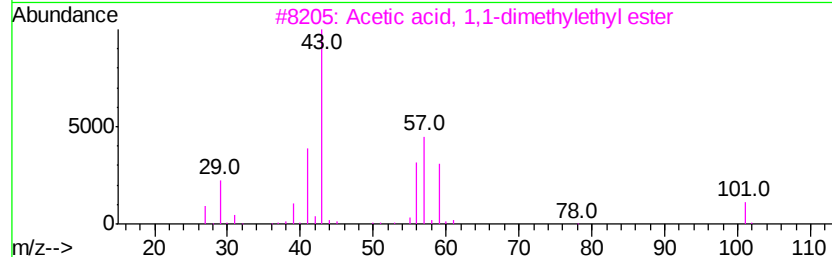
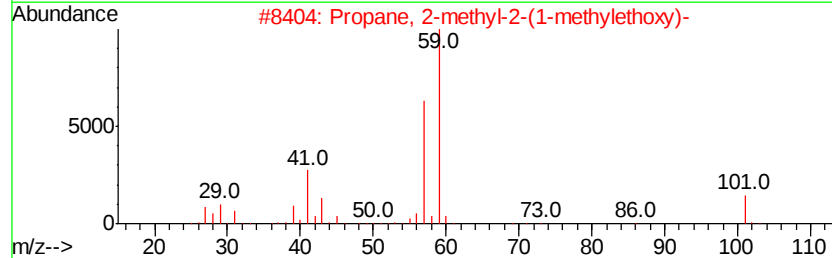
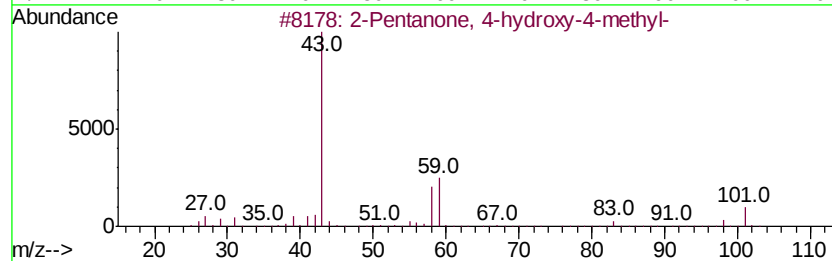
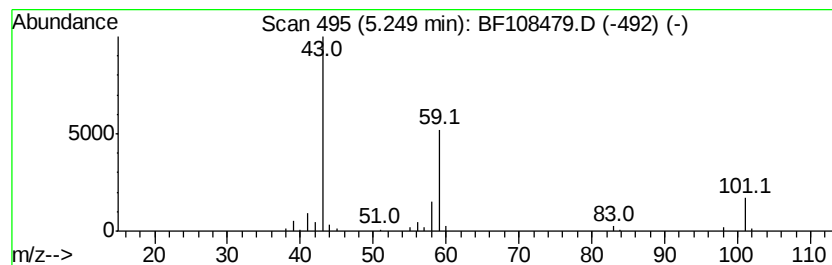
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	4.01 ng	176289	1,4-Dichlorobenzene-d4	7.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27



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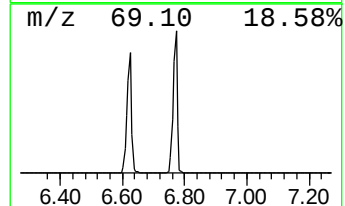
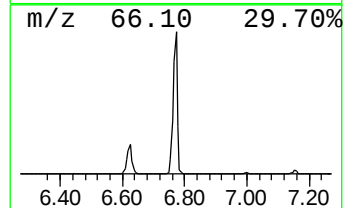
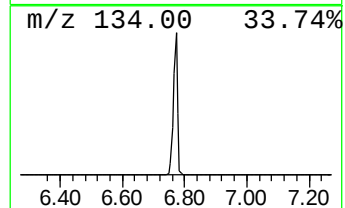
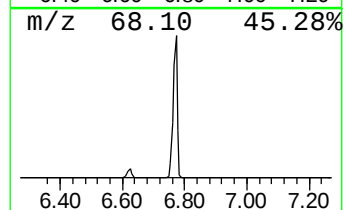
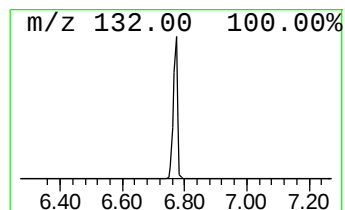
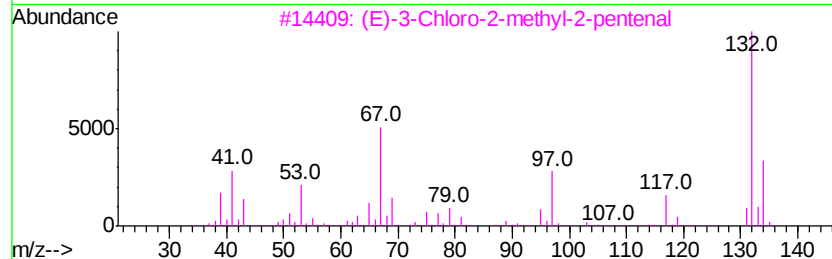
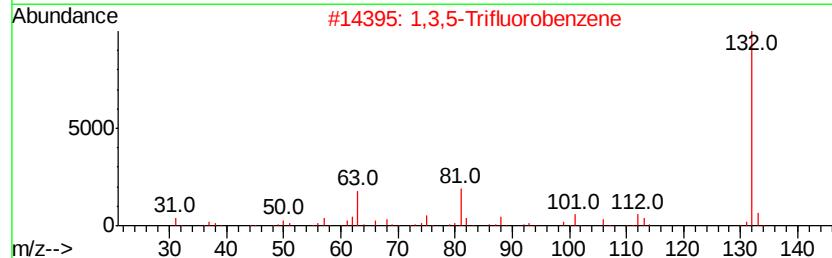
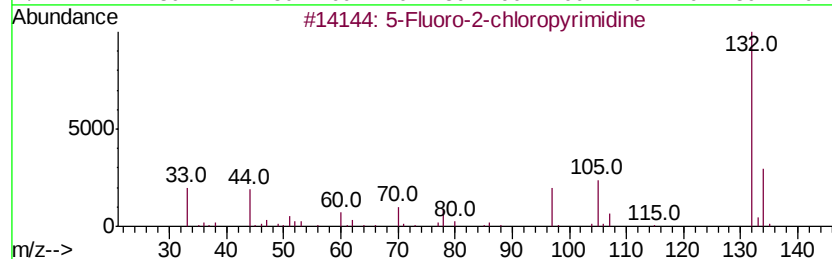
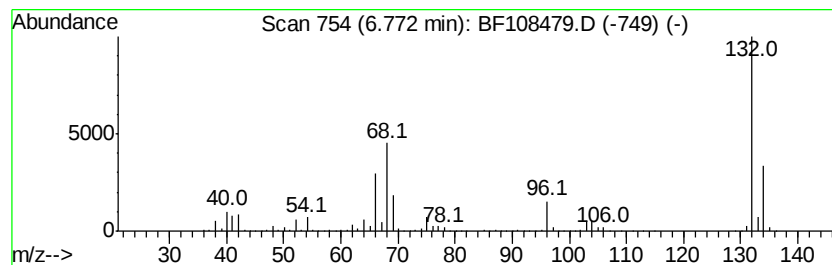
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Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	76.33 ng	3359410	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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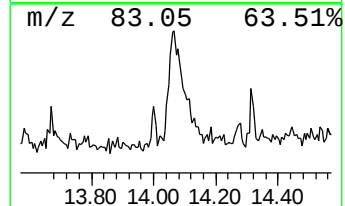
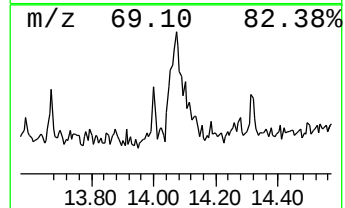
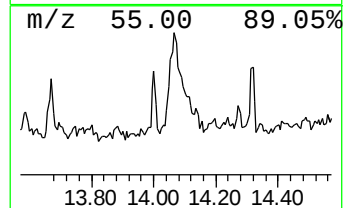
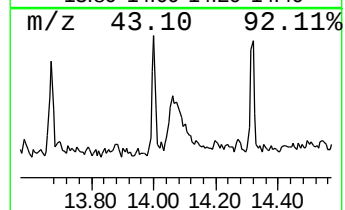
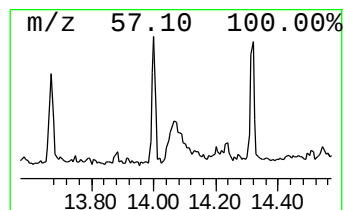
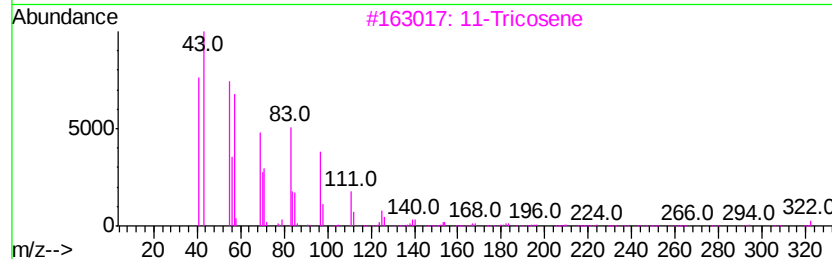
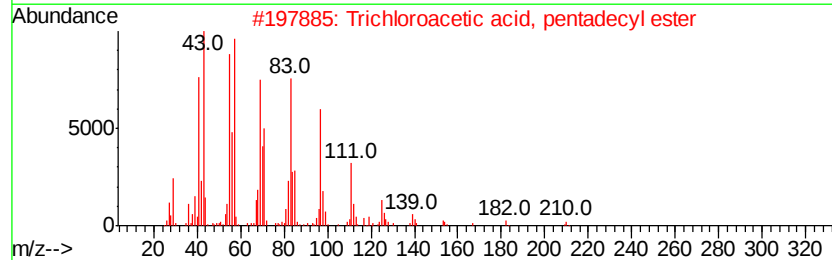
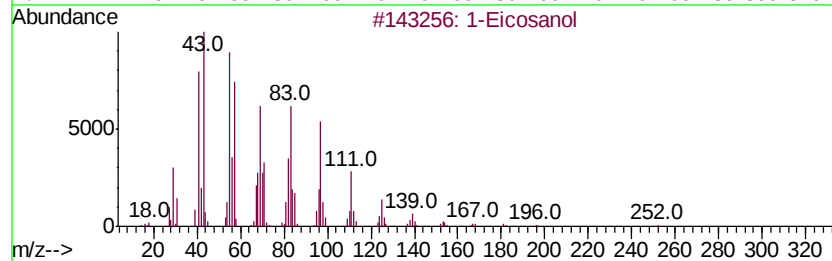
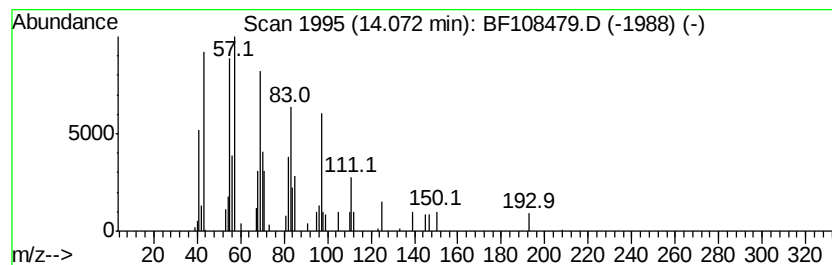
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Peak Number 5 1-Eicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	2.04 ng	85543	Chrysene-d12	14.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol		298	C20H42O	000629-96-9	91
2	Trichloroacetic acid, pentadecyl...		372	C17H31Cl3O2	074339-53-0	90
3	11-Tricosene		322	C23H46	052078-56-5	72
4	1-Hexacosanol		382	C26H54O	000506-52-5	43
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	43



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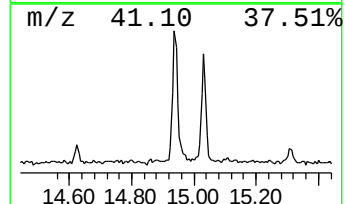
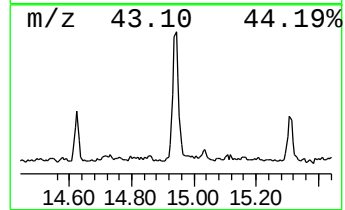
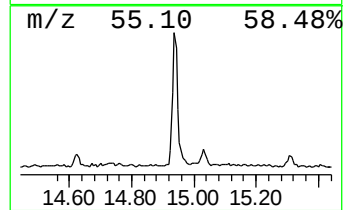
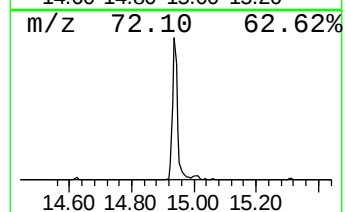
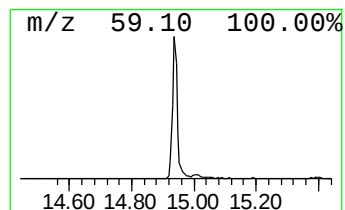
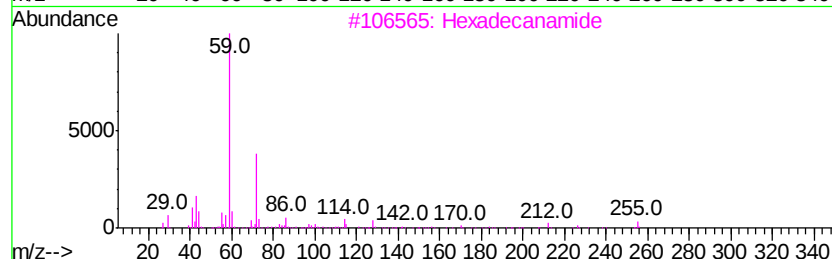
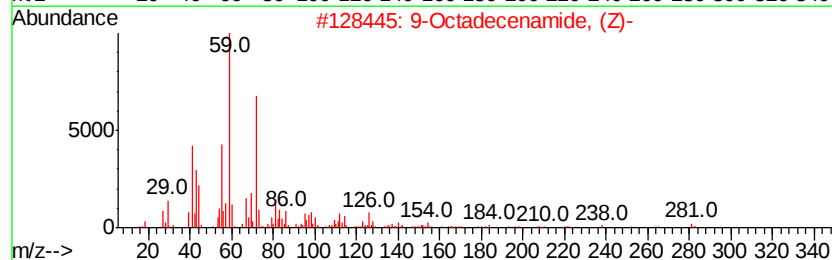
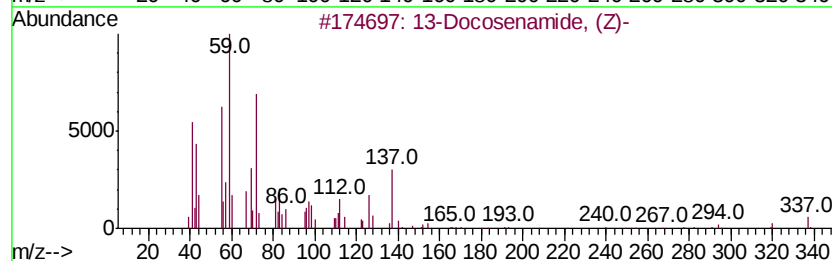
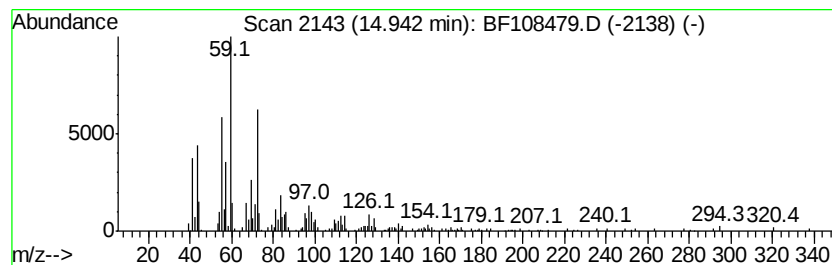
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 Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	10.53 ng	441682	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3		Hexadecanamide	255	C16H33NO	000629-54-9	78
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
5		Dodecanamide	199	C12H25NO	001120-16-7	59



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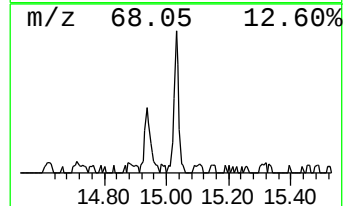
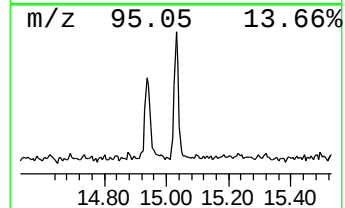
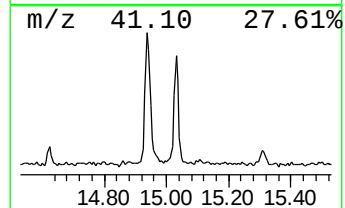
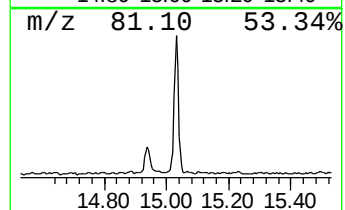
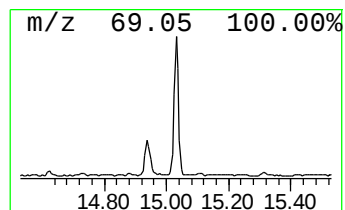
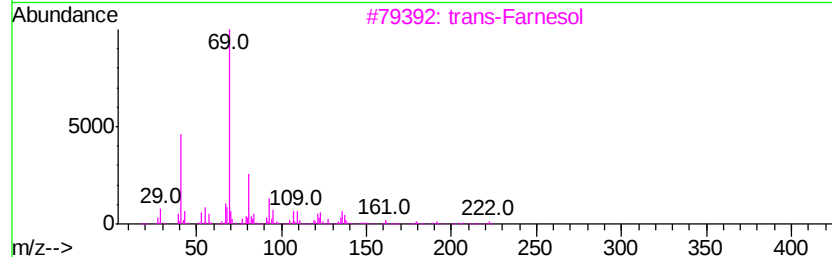
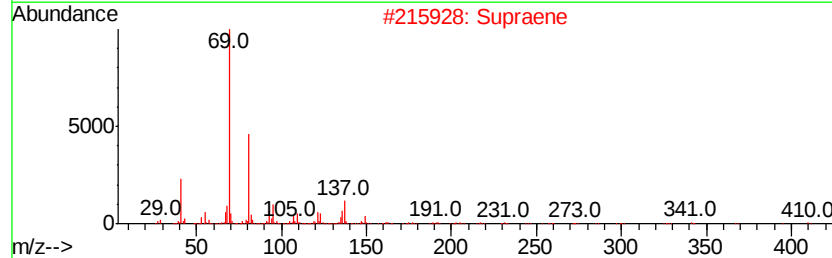
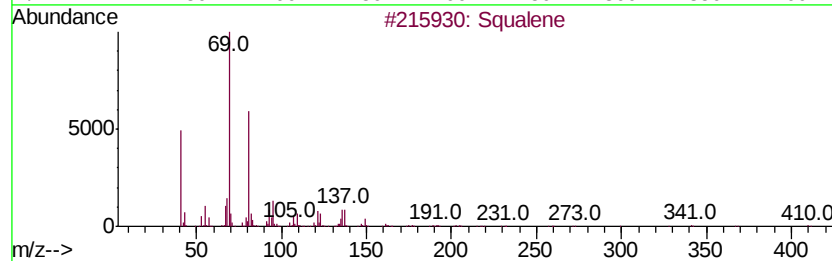
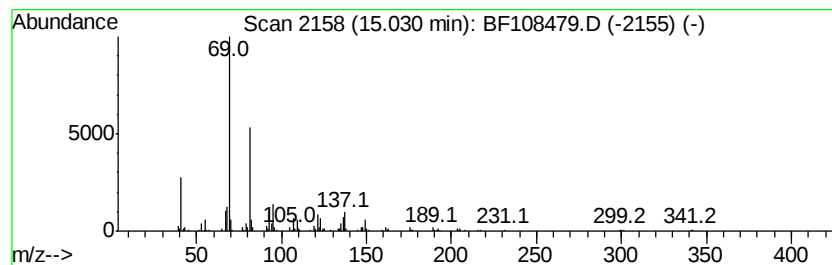
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	4.98 ng	216737	Perylene-d12	15.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		trans-Farnesol	222	C15H26O	000106-28-5	80
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082418\
Data File : BF108479.D
Acq On : 24 Aug 2018 22:29
Operator : JU/SJ
Sample : J4581-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q3-D1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.37	26.8	ng	1177700	1	7.00	880210	20.0
2-Pentanone, 4-hy...	5.25	4.0	ng	176289	1	7.00	880210	20.0
unknown6.77	6.77	76.3	ng	3359410	1	7.00	880210	20.0
1-Eicosanol	14.07	2.0	ng	85543	5	14.19	838854	20.0
13-Docosenamide, ...	14.94	10.5	ng	441682	5	14.19	838854	20.0
Squalene	15.03	5.0	ng	216737	6	15.74	870787	20.0